2,2-Dimethyl-1,3-dioxolane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -45.1 °C

Global applicability domain: Inside

Local applicability domain index: 6.17e-01

Confidence level: 3.67e-01

Nearest Neighbors from the Training Set

Image not found
tert-Butyl glycidyl ether
Measured: -70.0
Predicted: -69.5

Image not found
1,3-Dioxolane
Measured: -95.0
Predicted: -92.0

Image not found
Butanoic acid, ethenyl ester
Measured: 117
Predicted: 2.95

Image not found
Vinyl propionate
Measured: -80.0
Predicted: -69.2

Image not found
Ethyl acrylate
Measured: -71.2
Predicted: -69.2